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          and German available on STN
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FILE COVERS 1967 - 31 Aug 1999 VOL 131 ISS 10  
FILE LAST UPDATED: 31 Aug 1999 (19990831/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

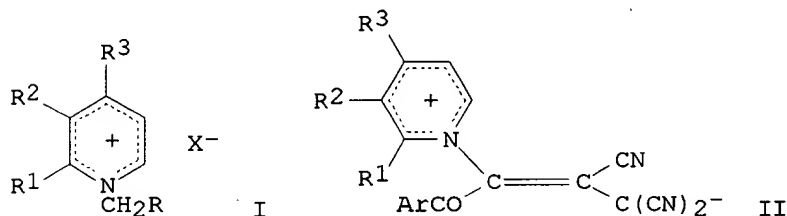
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=> s 11

L2 10 L1

=> d 1-10 iall

L2 ANSWER 1 OF 10 CAPLUS COPYRIGHT 1999 ACS  
ACCESSION NUMBER: 1991:655361 CAPLUS  
DOCUMENT NUMBER: 115:255361  
TITLE: Regioselectivity of reactions of azinium salts and ylides with tetracyanoethylene  
AUTHOR(S): Shestopalov, A. M.; Aitov, I. A.; Sharanin, Yu. A.; Litvinov, V. P.  
CORPORATE SOURCE: Inst. Org. Khim. im. Zelinskogo, Moscow, USSR  
SOURCE: Izv. Akad. Nauk SSSR, Ser. Khim. (1991), (6), 1431-9  
CODEN: IASKA6; ISSN: 0002-3353  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
CLASSIFICATION: 22-4 (Physical Organic Chemistry)  
OTHER SOURCE(S): CASREACT 115:255361  
GRAPHIC IMAGE:



ABSTRACT:

Reaction of azinium salts I [R = e.g., H, C<sup>6</sup>H<sub>5</sub>, CONH<sub>2</sub>; R<sub>1</sub>, R<sub>2</sub> = e.g., H, Me; (R<sub>1</sub>R<sub>2</sub>) = (CH:CH)<sub>2</sub>; R<sub>3</sub> = H, Me; X = halide, ClO<sub>4</sub><sup>-</sup>] with TCNE in aq. MeOH at 20.degree. proceeded by hydrolysis/anion exchange, with formation of I [X = -OC(CN):C(CN)<sub>2</sub>]. Azinium ylides generated in the reaction of I (R = COAr, Ar = substituted Ph; R<sub>1</sub>-R<sub>3</sub> = e.g., H, Me) with NEt<sub>3</sub> in MeOH reacted with TCNE via a stereoselective addn.-elimination reaction, forming Z 1,4-ylides II. The mechanism of reaction was discussed.

SUPPL. TERM: TCNE stereoselective addn elimination azinium salt; ylide  
aroylpyridiniumtricyanopropenide  
INDEX TERM: Hydrolysis  
(anion exchange and, in reaction of azinium salts with  
TCNE in aq. methanol)

INDEX TERM: Ylides  
 ROLE: PRP (Properties)  
 (aroylpyridiniotricyanopropenides, stereoselective  
 formation of, in reaction of azinium ylides with TCNE)

INDEX TERM: Addition reaction  
 (stereoselective, elimination and, in reaction of  
 azinium  
 ylides with TCNE)

INDEX TERM: 930-73-4 3947-76-0 10129-51-8 41220-29-5 52805-99-9  
 63008-23-1 78572-44-8 133828-84-9 136714-37-9  
 136714-38-0  
 ROLE: PRP (Properties)  
 (anion exchange/hydrolysis reaction of, with TCNE)

INDEX TERM: **16844-10-3** 16883-69-5 32896-98-3  
 ROLE: PRP (Properties)  
 (anion exchange/hydrolysis reaction of, with TCNE, and  
 stereoselective addn./elimination reaction of ylide  
 derived from, with TCNE)

INDEX TERM: 670-54-2, TCNE, reactions  
 ROLE: RCT (Reactant)  
 (hydrolysis/anion exchange reaction of, with azinium  
 salts, and stereoselective addn./elimination reaction  
 of,  
 with ylides derived from azinium salts)

INDEX TERM: 134720-91-5P 134720-92-6P 134720-95-9P 136714-39-1P  
 136714-40-4P 136714-41-5P 136714-43-7P 136714-44-8P  
 136714-46-0P 136714-48-2P 136714-50-6P 136714-51-7P  
 136714-53-9P 136714-54-0P 136714-57-3P 136714-58-4P  
 136714-59-5P 136714-60-8P 136714-61-9P 136714-62-0P  
 136714-63-1P 136714-64-2P 136714-65-3P 136714-66-4P  
 136974-27-1P  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

INDEX TERM: 7250-28-4 17282-37-0 25357-43-1 26031-66-3  
 82746-41-6 82746-43-8 136106-08-6 136714-55-1  
 136714-56-2  
 ROLE: PRP (Properties)  
 (stereoselective addn./elimination reaction of ylide  
 derived from, with TCNE)

L2 ANSWER 2 OF 10 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1990:478234 CAPLUS

DOCUMENT NUMBER: 113:78234

TITLE: New method of 1-pyrazoline ring formation

AUTHOR(S): Prostakov, N. S.; Varlamov, A. V.; Annan, Hussein;  
 Fomichev, A. A.; Aliev, A. E.

CORPORATE SOURCE: Univ. Druzhby Nar. im. P. Lumumby, Moscow, 117923,  
 USSR

SOURCE: Khim. Geterotsikl. Soedin. (1989), (12), 1697  
 CODEN: KGSSAQ; ISSN: 0453-8234

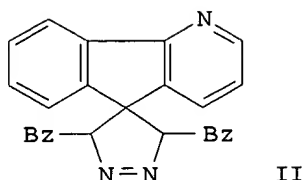
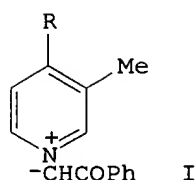
DOCUMENT TYPE: Journal

LANGUAGE: Russian

CLASSIFICATION: 28-8 (Heterocyclic Compounds (More Than One Hetero  
 Atom))

OTHER SOURCE(S): CASREACT 113:78234

GRAPHIC IMAGE:



# ABSTRACT:

Treating ylides I (R = Ph<sub>3</sub>Si, H), generated from the corresponding N-phenacylpyridinium bromides by aq. K<sub>2</sub>CO<sub>3</sub> in CHCl<sub>3</sub> at 20.degree., with 9-diazo-4-azafluorene in CHCl<sub>3</sub> for 5 h at 20.degree. gave 35 and 32% spiropyrazoline deriv. II.

SUPPL. TERM: phenacylpyridinium ylide diazotization cyclization; spirocarbazolepyrazole; pyrazole spirocarbazole  
 INDEX TERM: Ring closure and formation (of phenacylpyridine ylides with diazoazafluorene, spiro[azafluorene-pyrazoline] derivs. from)  
 INDEX TERM: Ylides  
 ROLE: RCT (Reactant) (of phenacylpyridines, cyclization by diazoazafluorene)  
 INDEX TERM: Spiro compounds  
 ROLE: SPN (Synthetic preparation); PREP (Preparation) (prepn. of spiro[azafluorene-pyrazoline] deriv.)  
 INDEX TERM: 50555-86-7  
 ROLE: RCT (Reactant) (cyclization by, of phenacylpyridine ylides, spiro[azafluorene-pyrazoline] derivs. from)  
 INDEX TERM: 56241-32-8 67433-80-1  
 ROLE: RCT (Reactant) (cyclization of, by diazoazafluorene, spiro[azafluorene-pyrazoline] deriv. from)  
 INDEX TERM: **16844-10-3** 67433-79-8  
 ROLE: RCT (Reactant) (generation of ylide from)  
 INDEX TERM: 128381-32-8P 128443-23-2P  
 ROLE: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

L2 ANSWER 3 OF 10 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1986:590862 CAPLUS

DOCUMENT NUMBER: 105:190862

TITLE: Stereochemical study on 1,3-dipolar cycloaddition reactions of heteroaromatic N-ylides with symmetrically substituted cis and trans olefins

AUTHOR(S): Tsuge, Otohiko; Kanemasa, Shuji; Takenaka, Shigeori  
 CORPORATE SOURCE: Interdiscip. Grad. Sch. Eng. Sci., Kyushu Univ., Kasuga, 816, Japan

SOURCE: Bull. Chem. Soc. Jpn. (1985), 58(11), 3137-57  
 CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 27-16 (Heterocyclic Compounds (One Hetero Atom))

OTHER SOURCE(S): CASREACT 105:190862

## ABSTRACT:

Stereochem. of the cycloaddns. of twenty-four heteroarom. N-ylides with sym. substituted cis and trans olefins has been investigated. Cyclic and acyclic cis olefins cycloadd to the anti form of the ylides in a highly endo-selective manner giving almost quant. yields of stereospecific endo 3+2 cycloadducts. N-Ylides stabilized with a substituent of the carbonyl type react with trans

olefins to form mostly 2 stereoisomeric 3+2 cycloadducts to the anti form of the ylides. In most cases, they undergo stereospecific interconversion through a retro cycloaddn. process, the isomer ratios and the ease of transformation depending upon the nature and size of substituents on the 5-membered ring which has been built up in the cycloaddn. step. On the other hand, N-ylides stabilized with a substituent of noncarbonyl type react with trans olefins to give stereospecific and stereoselective 3+2 cycloadducts as single isomers which are assigned as the cycloadducts to the syn form of the ylides.

SUPPL. TERM: ylide heteroarom olefin cycloaddn stereochem  
INDEX TERM: Cycloalkenes  
Alkenes, reactions  
ROLE: RCT (Reactant)  
(cycloaddn. of, with heteroarom. N-ylides, stereochem. of)  
INDEX TERM: Ylides  
ROLE: RCT (Reactant)  
(heteroarom. N-, cycloaddn. of, with olefins, stereochem. of)  
INDEX TERM: Stereochemistry  
(of cycloaddn. of heteroarom. N-ylides with olefins)  
INDEX TERM: Cycloaddition reaction  
(of heteroarom. N-ylides with olefins, stereochem. of)  
INDEX TERM: 762-42-5  
ROLE: PROC (Process)  
(addn. of, with diazatricyclododecadienes)  
INDEX TERM: 624-48-6 624-49-7 764-42-1 928-53-0 930-88-1  
941-69-5 959-27-3 959-28-4 1081-17-0 1631-28-3  
2973-17-3 7633-38-7 18305-60-7  
ROLE: PROC (Process)  
(cycloaddn. of, with heteroarom. N-ylides, stereochem. of)  
INDEX TERM: 108-31-6, reactions  
ROLE: RCT (Reactant)  
(cycloaddn. of, with heteroarom. N-ylides, stereochem. of)  
INDEX TERM: 289-80-5 946-07-6 4329-73-1 5304-34-7 7250-28-4  
7467-00-7 16726-82-2 **16844-10-3** 16883-69-5  
17282-40-5 17282-41-6 17282-43-8 18667-21-5  
25131-60-6 25357-39-5 25357-50-0 25357-51-1  
26489-32-7 32896-98-3 33014-32-3 39595-94-3  
40448-79-1 40448-80-4 51386-37-9 55814-00-1  
55841-58-2 56241-32-8 56567-29-4 57699-26-0  
58329-45-6 59456-80-3 59986-29-7 64636-81-3  
72797-44-5 72797-45-6 78113-64-1 80636-51-7  
82735-58-8 87773-11-3 88089-35-4 88089-43-4  
88089-46-7 90625-75-5 92171-46-5 104932-95-8  
104932-96-9 104932-97-0 104953-23-3 104953-24-4  
ROLE: PROC (Process)  
(cycloaddn. of, with olefins, stereochem. of)  
INDEX TERM: 104953-21-1P  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and oxidn. of)  
INDEX TERM: 37129-40-1P 78113-52-7P 78113-53-8P 78113-54-9P  
78184-05-1P 78184-06-2P 78184-07-3P 88089-36-5P  
88089-37-6P 88089-38-7P 88089-39-8P 88089-40-1P  
88089-41-2P 88089-44-5P 88089-45-6P 88121-62-4P  
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 105017-16-1P 105017-17-2P 105017-18-3P 105017-19-4P  
 105017-20-7P

ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

INDEX TERM: 100-48-1 110-86-1, reactions 119-65-3 288-47-1  
 591-22-0 3796-23-4

ROLE: RCT (Reactant)  
 (quaternization of)

INDEX TERM: 70-11-1 590-17-0 2114-00-3 15109-94-1

ROLE: RCT (Reactant)  
 (reaction of, with pyridine)

L2 ANSWER 4 OF 10 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1981:165607 CAPLUS

DOCUMENT NUMBER: 94:165607

TITLE: Pyridinium compound fogging agents for photographic material

INVENTOR(S): Oishi, Yasushi; Hirano, Shigeo

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan

SOURCE: Ger. Offen., 70 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

INT. PATENT CLASSIF.: G03C005-30

CLASSIFICATION: 74-2 (Radiation Chemistry, Photochemistry, and Photographic Processes)

Section cross-reference(s): 27

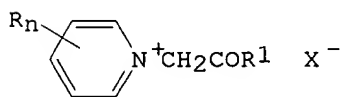
FAMILY ACC. NUM. COUNT: 1

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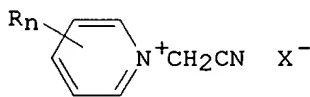
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3014628	A1	19801030	DE 1980-3014628	19800416
DE 3014628	C2	19910502		
JP 55138742	A2	19801029	JP 1979-46949	19790417
JP 62004699	B4	19870131		
US 4324855	A	19820413	US 1980-140923	19800416
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PRIORITY APPLN. INFO.:

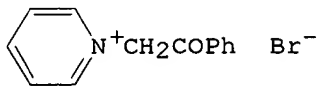
GRAPHIC IMAGE:



I



II



III

**ABSTRACT:**

Reversal images with a higher Dmax and a lower Dmin can be produced by incorporation of nucleating agents (fogging agents) of the formulas I or II (R = trihalomethyl, CN, carbamoyl, a carboxyl ester, carboxamido, sulfonamido, acyl, sulfonyl, sulfamoyl, acylamino, aryl, alkyl, or heterocycle; R1 = a mono-, di-, or tricyclic aryl group, a heterocycle, or a straight chain, branched chain, or cyclic alkyl; X- = anion; n = 0-3) into an internal latent image-forming emulsion layer contg. a dye-forming compd. and subsequently processing with an alk. soln. after imagewise exposure. Thus, a transparent cellulose acetate film support was coated with a layer contg. a magenta dye-releasing redox compd., a layer of a spectrally sensitized internal latent image-forming gelatin-AgBr emulsion contg. III 1.4 mmol/mol Ag, and a protective gelatin layer. This unit was then exposed, combined with a receptor element contg. a mordant, and processed with an alk. processing soln. to give a magenta pos. image with a Dmin of 0.03 and a Dmax of 1.25.

SUPPL. TERM: cyanoethylpyridinium fogging agent photog;  
aroylmethylpyridinium fogging agent photog;  
alkanoylmethylpyridinium fogging agent photog; pyridinium  
deriv fogging agent photog; nucleating agent pyridinium  
deriv photog; fogging agent pyridinium deriv photog

INDEX TERM: 5469-10-3 6277-72-1 6299-99-6 **16844-10-3**  
16844-14-7 16883-69-5 17281-59-3 17282-37-0  
17282-38-1 25357-39-5 25357-44-2 25357-46-4  
25407-31-2 26031-47-0 26031-59-4 26031-66-3  
26535-84-2 42508-60-1 49854-35-5 63374-35-6  
64881-07-8 69656-16-2 77281-09-5 77281-10-8  
77281-11-9 77281-12-0 77281-13-1 77281-14-2  
77281-15-3 77281-16-4 77281-17-5 77281-18-6  
77281-19-7 77281-20-0 77281-21-1 77281-22-2  
77281-23-3 77281-24-4 77281-25-5 77281-26-6  
77281-27-7 77281-28-8 77281-29-9 77281-30-2  
77281-31-3 77281-32-4 77281-33-5 77281-34-6  
77281-35-7

ROLE: USES (Uses)

(photog. fogging agent, for reversal image prodn.)

INDEX TERM: 29536-25-2P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation)

(prepn. and reaction of, with phenacyl bromide)

INDEX TERM: 20260-53-1

ROLE: RCT (Reactant)

(reaction of, with cetylamine)

INDEX TERM: 143-27-1

ROLE: RCT (Reactant)

(reaction of, with nicotinoyl chloride hydrochloride)

INDEX TERM: 70-11-1

ROLE: RCT (Reactant)

(reaction of, with N-hexadecylnicotinamide)

L2 ANSWER 5 OF 10 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1981:65440 CAPLUS

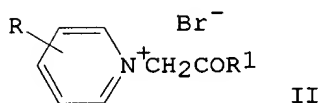
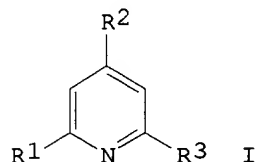
DOCUMENT NUMBER: 94:65440

TITLE: Studies on cycloimmonium ylides. Synthesis of some  
2,4,6-triaryl-substituted pyridines via picolinium  
ylides

AUTHOR(S): Tewari, Ram. S.; Dubey, Ajay K.; Misra, Naresh K.;  
Dixit, Priya D.

CORPORATE SOURCE: Dep. Chem., H. B. Technol. Inst., Kanpur, 208002,  
India

SOURCE: J. Chem. Eng. Data (1981), 26(1), 106-8  
 CODEN: JCEAAX; ISSN: 0021-9568  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 CLASSIFICATION: 27-17 (Heterocyclic Compounds (One Hetero Atom))  
 GRAPHIC IMAGE:

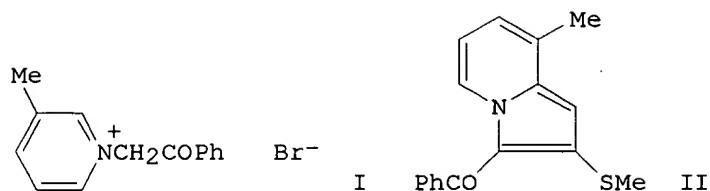


ABSTRACT:  
 2,4,6-Triaryl-substituted pyridines I were prepd. by reaction of  
 aroylmethylenepicolinium ylides II (R = 3-Me, 4-Me; R1 = Ph, 4-ClC6H4,  
 p-tolyl)  
 with R2CH:CHCOR3 (R2, R3 = optionally substituted Ph).

SUPPL. TERM: pyridine triphenyl; cyclocondensation picolinium ylide  
 chalcone  
 INDEX TERM: Cyclocondensation reaction  
 (of picolinium ylides with chalcones, substituted  
 pyridines from)  
 INDEX TERM: 94-41-7 959-23-9 1230-77-9 2373-89-9 2453-44-3  
 5416-71-7 6552-63-2 6552-66-5 6552-68-7 19133-00-7  
 19672-59-4 21551-47-3 42580-60-9 69538-64-3  
 72666-54-7 73911-01-0 75573-20-5 75573-21-6  
 ROLE: RCT (Reactant)  
 (cyclocondensation of, with picolinium ylides,  
 substituted pyridine from)  
 INDEX TERM: **16844-10-3** 25357-43-1 76337-69-4  
 ROLE: RCT (Reactant)  
 (cyclocondensation of, with substituted chalcones,  
 substituted pyridine from)  
 INDEX TERM: 580-35-8P 3557-65-1P 16112-42-8P 72666-41-2P  
 72666-42-3P 72666-45-6P 72666-47-8P 72666-48-9P  
 72666-49-0P 72666-50-3P 72673-14-4P 73910-87-9P  
 73910-89-1P 75573-10-3P 75573-11-4P 75573-12-5P  
 75573-13-6P 75573-14-7P 75573-15-8P  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

L2 ANSWER 6 OF 10 CAPLUS COPYRIGHT 1999 ACS  
 ACCESSION NUMBER: 1978:22552 CAPLUS  
 DOCUMENT NUMBER: 88:22552  
 TITLE: Reaction of pyridinium N-ylides with ketene  
 thioacetal  
 derivatives  
 AUTHOR(S): Tominaga, Yoshinori; Miyake, Yoshinori; Fujito,  
 Hiroshi; Kurata, Keiji; Awaya, Hiroyoshi; Matsuda,  
 Yoshiro; Kobayashi, Goro  
 CORPORATE SOURCE: Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, Japan  
 SOURCE: Chem. Pharm. Bull. (1977), 25(7), 1528-33  
 CODEN: CPBTAL  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 CLASSIFICATION: 27-17 (Heterocyclic Compounds (One Hetero Atom))  
 GRAPHIC IMAGE:





# ABSTRACT:

Reaction of the pyridinium N-ylides with ketenethioacetal in the presence of Et<sub>3</sub>N or K<sub>2</sub>CO<sub>3</sub> as a base in EtOH or DMF gave the pyridinium N-allylides which readily cyclized to give the indolizine derivs. Thus, the pyridinium ylide I and (MeS)2C:CHNO<sub>2</sub> gave the indolizine II.

SUPPL. TERM: pyridinium ylide reaction ketenethioacetal; indolizine  
 INDEX TERM: Cyclocondensation reaction

(of methylpyridinium ylides with ketene thioacetal  
 derivs., indolizine derivs. from)

INDEX TERM: Ylides

ROLE: RCT (Reactant)

(pyridinium, reaction of, with ketene thioacetal

derivs.)

INDEX TERM: 57845-14-4P 57845-15-5P 59182-01-3P 64908-40-3P  
 64908-43-6P 64995-24-0P 64995-25-1P 64995-26-2P  
 64995-27-3P 64995-28-4P 64995-29-5P 64995-30-8P  
 64995-31-9P 64995-32-0P 64995-33-1P 64995-34-2P  
 64995-35-3P 64995-36-4P 64995-37-5P 64995-38-6P

ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

INDEX TERM: 7250-28-4 16844-10-3 16883-69-5 17282-40-5  
 41220-29-5 56567-29-4 64636-79-9 64636-80-2  
 64995-39-7 64995-40-0 64995-41-1 64995-42-2  
 64995-43-3

ROLE: RCT (Reactant)  
 (reaction of, with ketenethioacetals)

INDEX TERM: 3490-92-4 5147-80-8 13623-94-4 17823-58-4  
 18374-66-8

ROLE: RCT (Reactant)  
 (reaction of, with pyridinium ylides)

L2 ANSWER 7 OF 10 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1977:601268 CAPLUS

DOCUMENT NUMBER: 87:201268

TITLE: Heterocyclic ketene thioacetal derivatives. VIII.  
 Synthesis of ketene thioacetals having a pyridinium  
 salt

AUTHOR(S): Tominaga, Yoshinori; Miyake, Yoshinori; Fujito,  
 Hiroshi; Matsuda, Yoshiro; Kobayashi, Goro

CORPORATE SOURCE: Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, Japan

SOURCE: Yakugaku Zasshi (1977), 97(8), 927-32

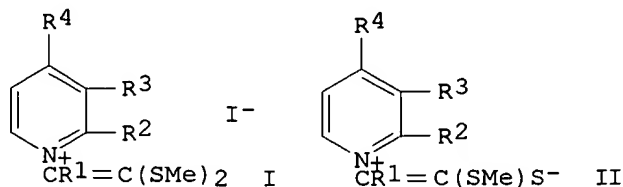
CODEN: YKKZAJ

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

CLASSIFICATION: 27-17 (Heterocyclic Compounds (One Hetero Atom))

GRAPHIC IMAGE:



**ABSTRACT:**

Ketenethioacetal derivs. I ( $R_1 = \text{Bz}, \text{CO}_2\text{Et}, \text{CONH}_2, \text{CN}$ ;  $R_2, R_3, R_4 = \text{H}, \text{Me}$ ) were prepd. by alkylation with MeI of II, which were prepd. by the reaction of pyridinium ylides with  $\text{CS}_2$  in the presence of NaOH.

SUPPL. TERM: pyridinium ketene thioacetal deriv; ylide pyridinium  
reaction carbon disulfide

INDEX TERM: Mercaptals and Mercaptoles  
ROLE: RCT (Reactant)  
(ketene thioacetals with a pyridinium salt)

INDEX TERM: Ylides  
ROLE: RCT (Reactant)  
(pyridinium, reaction of, with carbon disulfide)

INDEX TERM: 64636-63-1P 64636-64-2P 64636-65-3P 64636-66-4P  
64636-67-5P 64636-68-6P 64636-69-7P 64636-70-0P  
64636-71-1P 64636-72-2P 64636-73-3P 64636-74-4P  
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation)  
(prepn. and reaction with methyl iodide)

INDEX TERM: 57845-27-9P 59181-92-9P 59181-93-0P 59181-94-1P  
59181-95-2P 59181-96-3P 59181-97-4P 59181-98-5P  
64636-75-5P 64636-76-6P 64636-82-4P 64636-83-5P  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

INDEX TERM: 7250-28-4 **16844-10-3** 17282-40-5 26557-57-3  
32896-98-3 42866-67-1 55814-02-3 64636-77-7  
64636-78-8 64636-79-9 64636-80-2 64636-81-3  
ROLE: RCT (Reactant)  
(reaction of, with carbon disulfide and dimethyl  
sulfate)

INDEX TERM: 75-15-0, reactions  
ROLE: RCT (Reactant)  
(reaction of, with pyridinium ylides)

INDEX TERM: 74-88-4, reactions 75-18-3  
ROLE: RCT (Reactant)  
(reaction of, with sulfur contg. pyridinium ylides)

L2 ANSWER 8 OF 10 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1975:514165 CAPLUS

DOCUMENT NUMBER: 83:114165

TITLE: Route to 2,6-dihydroxypiperidines

AUTHOR(S): Wild, Peter; Kroehnke, Fritz

CORPORATE SOURCE: Inst. Org. Chem., Univ. Giessen, Giessen, Ger.

SOURCE: Justus Liebigs Ann. Chem. (1975), (5), 849-63

CODEN: JLACBF

DOCUMENT TYPE: Journal

LANGUAGE: German

CLASSIFICATION: 27-17 (Heterocyclic Compounds (One Hetero Atom))

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.

**ABSTRACT:**

Acylalkylpyridinium salts I ( $R = \text{H}, 3\text{-Me}, 4\text{-Me}, 3,5\text{-Me}_2$ ;  $R_1 = \text{Me}, \text{Ph}, 4\text{-MeC}_6\text{H}_4$ )

reacted with R2CHO (R2 = H, Ph, 4-MeC6H4) and R3NH2 (R3 = H, Me) in a 2:1:1 molar ratio to give .apprx.60% dipyridinium salts II. II lost 1 mole H2O to give tetrahydro derivs. III and a 2nd mole H2O to give dihydro derivs. IV. IV were dehydrogenated to the corresponding pyridine compds. which were readily ring-cleaved to give pyridinediamines V and glutaconaldehyde deriv. VI. Excess piperidine causes chain-shortening of VI.

SUPPL. TERM: acylpyridinium reaction aldehyde ammonia; pyridinium acyl reaction aldehyde ammonia; amine reaction acylpyridinium; hydroxypiperidinediyl dipyridinium; piperidinediyl dipyridinium dihydroxy; glutaconaldehyde Schiff base; dehydration

dihydroxypiperidinediyl dipyridinium

INDEX TERM: Dehydration, chemical (acid-catalyzed, of (dihydroxypiperidinediyl) dipyridinium salts)

INDEX TERM: Aldehydes, reactions

ROLE: RCT (Reactant) (with acylalkylpyridinium salts and ammonia)

INDEX TERM: 56566-74-6P 56566-75-7P 56566-76-8P 56566-77-9P 56566-78-0P 56566-81-5P 56566-82-6P 56566-83-7P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and dehydration of)

INDEX TERM: 56566-87-1P 56566-89-3P 56566-91-7P 56566-93-9P 56566-97-3P 56567-05-6P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and dehydrogenation of)

INDEX TERM: 56567-15-8P 56567-17-0P 56567-19-2P 56567-21-6P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and ring cleavage of)

INDEX TERM: 2473-39-4P 2473-40-7P 56566-80-4P 56566-85-9P 56566-95-1P 56566-99-5P 56567-01-2P 56567-03-4P 56567-07-8P 56567-09-0P 56567-11-4P 56567-13-6P 56567-23-8P 56567-25-0P 56567-26-1P 56567-27-2P 56567-28-3P 56567-30-7P 56567-31-8P 56567-32-9P 56567-34-1P 56567-36-3P

ROLE: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

INDEX TERM: 16883-69-5

ROLE: RCT (Reactant) (reaction with aldehydes and ammonia or methylamine)

INDEX TERM: 7250-28-4 16844-10-3 56567-29-4

ROLE: RCT (Reactant) (reaction with benzaldehyde and ammonia)

INDEX TERM: 17282-38-1 17282-41-6

ROLE: RCT (Reactant) (reaction with methylbenzaldehyde and ammonia)

INDEX TERM: 104-87-0

ROLE: RCT (Reactant) (reaction with phenacyl- or acetonylpyridinium bromides and ammonia)

INDEX TERM: 74-89-5

ROLE: RCT (Reactant) (reaction with phenacylpyridinium bromide and benzaldehyde)

INDEX TERM: 7664-41-7, reactions

ROLE: RCT (Reactant) (with phenacyl- or acetonylpyridinium bromides and

aldehydes)  
INDEX TERM: 100-52-7, reactions  
ROLE: RCT (Reactant)  
(with phenacyl- or acetonylpyridinium bromides and ammonia or methylamine)  
INDEX TERM: 50-00-0, reactions  
ROLE: RCT (Reactant)  
(with phenacylpyridinium bromide and ammonia)

L2 ANSWER 9 OF 10 CAPLUS COPYRIGHT 1999 ACS  
ACCESSION NUMBER: 1974:36969 CAPLUS  
DOCUMENT NUMBER: 80:36969  
TITLE: Synthesis and thermal reaction of pyridinium 3,3-diacyl-1-benzoylallylides[3,3-diacyl-1-benzoyl-1-(1-pyridinio)prop-2-enides]. Formation of indolizine derivatives  
AUTHOR(S): Tamura, Yasumitsu; Sumida, Yoshio; Ikeda, Masazumi  
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, Japan  
SOURCE: J. Chem. Soc., Perkin Trans. 1 (1973), (19), 2091-5  
CODEN: JCPRB4  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
CLASSIFICATION: 27-17 (Heterocyclic Compounds (One Hetero Atom))  
GRAPHIC IMAGE: For diagram(s), see printed CA Issue.  
ABSTRACT: Pyridinium phenacylides with 2,2-diacyl-1-ethoxyethylenes gave pyridinium 3,3-diacyl-1-benzoyl-allylides. E.g. pyridinium phenacylide with EtOCH:C(COMe)<sub>2</sub> gave 75% allylide (I, R = H). I (R = H) in refluxing Me<sub>2</sub>C<sub>6</sub>H<sub>4</sub> gave 6% indolizine (II; R = H, R<sub>1</sub> = Bz). 2-Methyl derivs. of I in refluxing Me<sub>2</sub>C<sub>6</sub>H<sub>4</sub> gave mainly 1-acetyl-2-phenylindolizines. E.g. I (R = Me) gave 30% II (R = Ph, R<sub>1</sub> = CH:CHCOMe) and 2% II (R = H, R<sub>1</sub> = Bz).

SUPPL. TERM: pyridinium allylide; pyridiniopropenide; propenide  
pyridinio; cyclization pyridinium allylide indolizine  
INDEX TERM: Ring closure and formation  
(of pyridinium diacylbenzoylallylides, indolizines by)  
INDEX TERM: 70-11-1  
ROLE: PROC (Process)  
(cycloaddn. of, with acetonylpyridine)  
INDEX TERM: 7250-28-4 **16844-10-3** 16883-69-5  
ROLE: PROC (Process)  
(cycloaddn. of, with acetylacetylene)  
INDEX TERM: 6302-02-9  
ROLE: PROC (Process)  
(cycloaddn. of, with phenacyl bromide)  
INDEX TERM: 1423-60-5  
ROLE: PROC (Process)  
(cycloaddn. of, with phenacylpyridinium bromide)  
INDEX TERM: 51386-31-3P 51386-32-4P 51386-33-5P 51386-34-6P  
51386-35-7P 51386-36-8P 51386-40-4P 51386-41-5P  
51386-42-6P 51386-43-7P 51386-44-8P 51386-45-9P  
51386-46-0P 51386-47-1P 51386-48-2P 51386-49-3P  
ROLE: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)  
INDEX TERM: 17282-43-8 25357-50-0 51386-37-9 51386-38-0  
51386-39-1  
ROLE: RCT (Reactant)  
(reaction of, with (ethoxymethylene)pentanedione)  
INDEX TERM: 87-13-8 94-05-3 33884-41-2  
ROLE: RCT (Reactant)  
(reaction of, with pyridinium phenacylides)

L2 ANSWER 10 OF 10 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1967:453263 CAPLUS  
 DOCUMENT NUMBER: 67:53263  
 TITLE: Kinetics of the reaction of pyridines with phenacyl bromide in nitrobenzene  
 AUTHOR(S): Litvinenko, L. M.; Perel'man, L. A.  
 CORPORATE SOURCE: Donetsk. Gos. Univ., Donetsk, USSR  
 SOURCE: Zh. Org. Khim. (1967), 3(5), 936-42  
 CODEN: ZORKAE  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 CLASSIFICATION: 22 (Physical Organic Chemistry)  
 ABSTRACT:

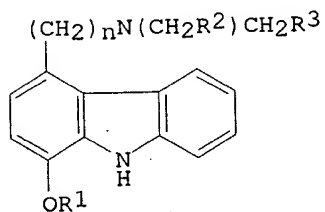
The title reaction was found to proceed irreversibly and nearly quant. with formation of compds. of general formula  $(RC_5H_4N+CH_2Bz)Br^-$  (I), where  $RC_5H_4N$  is substituted pyridine. The reaction kinetics were followed by potentiometric titrn. of the appearing  $Br^-$ . Rate consts. (k), activation energies (E), entropy changes ( $\Delta S$ ), and log A (A frequency factor) were calcd. Also Hammett-Taft consts.,  $\sigma$  and  $\rho$ , were detd. from the equation  $\log KR - \log KH = \rho \cdot \sigma$  (R, m.p.,  $\sigma$ , K at 25°, K at 40°, K at 55° in 1. mole<sup>-1</sup> sec.<sup>-1</sup> times 10<sup>3</sup>, E in cal. mole<sup>-1</sup>, S in cal. degree<sup>-1</sup> mole<sup>-1</sup>, log A in 1. mol.<sup>-1</sup> sec.<sup>-1</sup> given) 0 H, 206.5°, 0, 1.93  $\pm$  0.04, 4.80  $\pm$  0.16, 12.6  $\pm$  0.5, 11,900, -33.8, 6.01; 3-Me, 189-90°, -0.07, 4.84  $\pm$  0.03, 10.2  $\pm$  0.2, 22.9  $\pm$  0.7, 11,000, -34.5, 5.65; 3-NO<sub>2</sub>, 201-2°, 0.70, 0.00338  $\pm$  0.00014, 0.0104  $\pm$  0.0001, 0.0289  $\pm$  0.0002, 13,900, -39.7, 4.73; 3-Br, 194-5°, 0.38, 0.0660  $\pm$  0.0011, 0.185  $\pm$  0.008, 0.472  $\pm$  0.010, 12,800, -37.6, 5.18; 4-Et, 218-19°, -0.15, 5.83  $\pm$  0.14, 15.2  $\pm$  0.7, 32.0  $\pm$  0.8, 11,100, -34.3, 5.89; 4-NH<sub>2</sub>, 299-300°, -0.38, 179.0  $\pm$  0.6, 378.0  $\pm$  17.0, 729.0  $\pm$  25.0, 9100, -34.1, 5.95; 3-Bz, 238-40°, 0.34, 0.170  $\pm$  0.003, -, -, -, -, -; 4-Ph, 203-5°, 0, 2.63  $\pm$  0.13, 6.55  $\pm$  0.10, 14.8  $\pm$  0.7, 11,200, -35.5, 5.64.

SUPPL. TERM: HAMMETT TAFT KINETICS; PHENACYL BROMIDE PYRIDINES KINETICS; PYRIDINES KINETICS PHENACYL BROMIDE  
 INDEX TERM: Activation energy  
 Frequency factor  
 (of 2-bromoacetophenone reaction with pyridines)  
 INDEX TERM: Kinetics, reaction  
 (of 2-bromoacetophenones with pyridines)  
 INDEX TERM: Entropy  
 (of activation, of 2-bromoacetophenone reaction with pyridines)  
 INDEX TERM: 6299-99-6P **16844-10-3P** 16844-11-4P 16844-13-6P  
 16844-14-7P 16844-15-8P 16883-69-5P 16883-70-8P  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 INDEX TERM: 108-99-6 504-24-5 536-75-4 626-55-1 939-23-1  
 2530-26-9 5424-19-1  
 ROLE: PRP (Properties)  
 (reaction with 2-bromoacetophenone, kinetics of)  
 INDEX TERM: 70-11-1  
 ROLE: PRP (Properties)  
 (reaction with pyridines, kinetics of)  
 INDEX TERM: 110-86-1, reactions  
 ROLE: RCT (Reactant)  
 (with 2-bromoacetophenone, kinetics of)

preparation); PREP (Preparation)  
 (process for the prepn. of benzothiazolones)  
 IT 108773-04-2P  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (process for the prepn. of benzothiazolones)  
 IT 55-81-2 532-55-8, Benzoylisothiocyanate  
 RL: RCT (Reactant)  
 (process for the prepn. of benzothiazolones)

L17 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 1999 ACS  
 AN 1993:495333 HCAPLUS  
 DN 119:95333  
 TI Preparation of carbazoles as dopaminergic receptor antagonists  
 IN Hibino, Satoshi; Okuyama, Shigeru; Nakazato, Atsuo; Kawashima, Yutaka  
 PA Taisho Pharma Co Ltd, Japan  
 SO Jpn. Kokai Tokkyo Koho, 7 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 IC ICM C07D209-88  
 ICS A61K031-40  
 CC 27-11 (Heterocyclic Compounds (One Hetero Atom))  
 Section cross-reference(s): 1  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05058998	A2	19930309	JP 1991-226856	19910906
OS	MARPAT 119:95333				
GI					



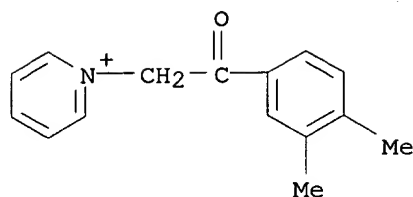
I

AB Carbazoles I ( $R^1 = H$ , C1-5 alkyl;  $R^2, R^3 = C1-5$  alkyl;  $n = 1-3$ ) and their salts, useful for treatment of aggressive behaviors, excitement, etc., in cerebrovascular disorders and senile dementia, are prepd. Treatment of 0.79 g 1-methoxy-4-(N-propyl-N-propionyl)aminoethylcarbazole (prepn. given) with  $LiAlH_4$  in THF at room temp. for 14 h gave 0.71 g I ( $R^1 = Me$ ,  $R^2 = R^3 = Et$ ,  $n = 2$ ) (II), which was converted into HCl salt in 75.4% yield. II inhibited specific binding of (-)-[3H]-sulpiride to adrenergic D2 receptor with  $IC_{50}$  of 648 nM, vs. 86,000 nM, for rimcazole.

ST adrenergic receptor antagonist carbazole prepn; cerebrovascular disorder dementia treatment carbazole

IT Adrenergic antagonists  
 (carbazoles, for treatment of cerebrovascular disorders and senile dementia)

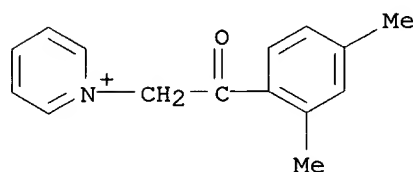
IT Mental disorder  
 (treatment of, carbazoles for)



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2 REFERENCES IN FILE CA (1967 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L6 ANSWER 2 OF 4 REGISTRY COPYRIGHT 1999 ACS  
RN 59224-30-5 REGISTRY  
CN **Pyridinium, 1-[2-(2,4-dimethylphenyl)-2-oxoethyl]-, bromide (9CI)**  
(CA INDEX NAME)  
MF **C15 H16 N O . Br**  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, TOXLIT  
(\*File contains numerically searchable property data)



● Br<sup>-</sup>

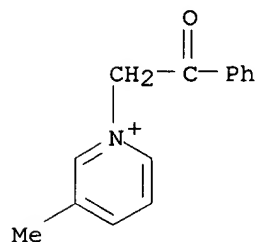
2 REFERENCES IN FILE CA (1967 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L6 ANSWER 3 OF 4 REGISTRY COPYRIGHT 1999 ACS  
RN 56567-29-4 REGISTRY  
CN **Pyridinium, 3,5-dimethyl-1-(2-oxo-2-phenylethyl)-, bromide (9CI)**  
(CA INDEX NAME)  
OTHER NAMES:  
CN **3,5-Dimethyl-1-phenacylpyridinium bromide**  
MF **C15 H16 N O . Br**  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT  
(\*File contains numerically searchable property data)  
CRN (110854-02-9)



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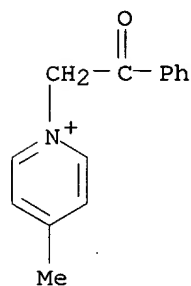
CN 1-Phenacyl-3-picolinium bromide  
CN **3-Methyl-1-phenacylpyridinium bromide**  
MF **C14 H14 N O . Br**  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, USPATFULL  
(\*File contains numerically searchable property data)  
CRN (59036-97-4)



● Br<sup>-</sup>

10 REFERENCES IN FILE CA (1967 TO DATE)  
10 REFERENCES IN FILE CAPLUS (1967 TO DATE)

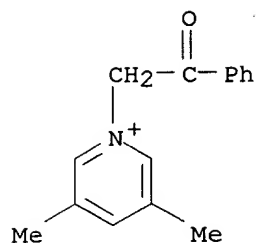
L3 ANSWER 4 OF 5 REGISTRY COPYRIGHT 1999 ACS  
RN 7250-28-4 REGISTRY  
CN **Pyridinium, 4-methyl-1-(2-oxo-2-phenylethyl)-, bromide (9CI)**  
(CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN 1-Phenacyl-4-picolinium bromide (6CI)  
CN 4-Picolinium, 1-phenacyl-, bromide (8CI)  
OTHER NAMES:  
CN **1-Phenacyl-4-methylpyridinium bromide**  
CN **4-Methyl-1-phenacylpyridinium bromide**  
MF **C14 H14 N O . Br**  
LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, IFICDB, IFIPAT,  
IFIUDB, TOXLIT, USPATFULL  
(\*File contains numerically searchable property data)  
CRN (46720-78-9)



● Br<sup>-</sup>

22 REFERENCES IN FILE CA (1967 TO DATE)  
22 REFERENCES IN FILE CAPLUS (1967 TO DATE)  
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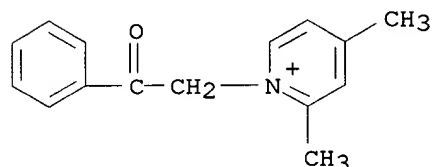




● Br<sup>-</sup>

6 REFERENCES IN FILE CA (1967 TO DATE)  
6 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L6 ANSWER 4 OF 4 REGISTRY COPYRIGHT 1999 ACS  
RN 26557-57-3 REGISTRY  
CN **Pyridinium, 2,4-dimethyl-1-(2-oxo-2-phenylethyl)-, bromide (9CI)**  
(CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN **Pyridinium, 2,4-dimethyl-1-phenacyl-, bromide (8CI)**  
MF **C15 H16 N O . Br**  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CHEMINFORMRX  
(\*File contains numerically searchable property data)



● Br<sup>-</sup>

3 REFERENCES IN FILE CA (1967 TO DATE)  
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> s 56567-29-4/rn

L7 1 56567-29-4/RN

=> s 16844-10-3/rn

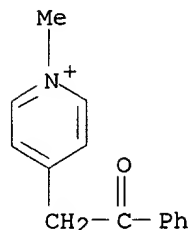
L8 1 16844-10-3/RN

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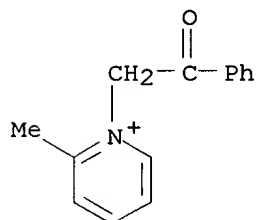
LC STN Files: BEILSTEIN\*, CA, CAPLUS  
(\*File contains numerically searchable property data)  
CRN (188903-44-8)



● Br<sup>-</sup>

1 REFERENCES IN FILE CA (1967 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)


L3 ANSWER 2 OF 5 REGISTRY COPYRIGHT 1999 ACS  
RN 32896-98-3 REGISTRY  
CN **Pyridinium, 2-methyl-1-(2-oxo-2-phenylethyl)-, bromide (9CI)**  
(CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN 2-Picolinium, 1-phenacyl-, bromide (8CI)  
OTHER NAMES:  
CN **2-Methyl-1-phenacylpyridinium bromide**  
CN **2-Methyl-N-phenacylpyridinium bromide**  
MF **C14 H14 N O . Br**  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX,  
CSCHEM  
(\*File contains numerically searchable property data)  
CRN (136714-42-6)



● Br<sup>-</sup>

18 REFERENCES IN FILE CA (1967 TO DATE)  
18 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L3 ANSWER 3 OF 5 REGISTRY COPYRIGHT 1999 ACS  
RN 16844-10-3 REGISTRY  
CN **Pyridinium, 3-methyl-1-(2-oxo-2-phenylethyl)-, bromide (9CI)**  
(CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN 3-Picolinium, 1-phenacyl-, bromide (8CI)  
OTHER NAMES:  
CN **1-Phenacyl-3-methylpyridinium bromide**



IT Cardiovascular system  
(disease, treatment of, carbazoles for)

IT Mental disorder  
(senile psychosis, treatment of, carbazoles for)

IT 79-03-8, Propionyl chloride  
RL: RCT (Reactant)  
(amidation of, with methoxyphenethylamine)

IT 55-81-2, 4-Methoxyphenethylamine  
RL: RCT (Reactant)  
(amidation of, with propionyl chloride)

IT 577-19-5, o-Nitrobromobenzene  
RL: RCT (Reactant)  
(condensation of, with aminophenethylamine deriv.)

IT 67191-51-9P 102842-44-4P 149081-92-5P **149081-93-6P**  
**149081-94-7P** 149081-95-8P 149081-96-9P 149081-97-0P  
149081-98-1P 149081-99-2P 149082-00-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and reaction of)

IT 149060-88-8P 149082-01-9P 149082-02-0P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, for treatment of cerebrovascular disorders and senile dementia)

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 13, 1999

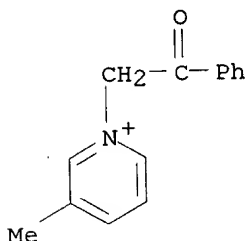
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L1 1 16844-10-3/RN

=> d

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 1999 ACS  
 RN 16844-10-3 REGISTRY  
 CN Pyridinium, 3-methyl-1-(2-oxo-2-phenylethyl)-, bromide (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN 3-Picolinium, 1-phenacyl-, bromide (8CI)  
 OTHER NAMES:  
 CN 1-Phenacyl-3-methylpyridinium bromide  
 CN 1-Phenacyl-3-picolinium bromide  
 CN 3-Methyl-1-phenacylpyridinium bromide  
 MF C14 H14 N O . Br  
 LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT, USPATFULL  
 (\*File contains numerically searchable property data)  
 CRN (59036-97-4)



● Br<sup>-</sup>

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Et, R = Ph) with NH<sub>4</sub>OH and refluxing Me<sub>2</sub>CHOH gave Et 2-phenyl-7-indolizinecarboxylate (IV). Acylation of III and IV by Ac<sub>2</sub>O, BzCl, and 4-ClC<sub>6</sub>H<sub>4</sub>COCl yielded the acylindolizines V (R<sub>2</sub> = Me, Ph; R<sub>3</sub> = Me, Ph, 4-ClC<sub>6</sub>H<sub>4</sub>).

IT **54342-81-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and cyclization of)

L14 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 1999 ACS

AN 1970:77111 HCAPLUS

DN 72:77111

TI Further structure-activity relations of heterocyclic analogs of hemicholinium 3

AU Benz, Frederick W.; Long, John Paul

CS Dep. of Pharmacol., Univ. of Iowa, Iowa City, Iowa, USA

SO J. Pharm. Pharmacol. (1970), 22(1), 20-5

CODEN: JPPMAB

DT Journal

LA English

AB The importance of the 3-Me group on the pyridinium ring of bis-quaternary nitrogen salts for hemicholinium-3-like activity having been conditionally established (Benz and Long, 1969), derivs. contg. classical isosteres of the 3-Me group and the 3 oxidn. states of the 3-Me group were examd. Oxidn. of the 3-Me group to CH<sub>2</sub>OH decreased activity tenfold. Subsequent oxidn. to CHO and CO<sub>2</sub>H further decreased activity. When the 3-Me group was replaced by a halogen, activity was maintained by the iodo-deriv. but decreased as the size of the halogen decreased and as the electronegativity increased. Substitution of an Et group for the 3-Me decreased activity twofold, whereas replacement with OH eliminated activity.

IT **24620-81-3**

RL: BIOL (Biological study)  
(neuromuscular inhibition by)